REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
01/09/2017

2. REPORT TYPE
Briefing Charts

3. DATES COVERED *(From - To)*
01 January 2017 - 31 January 2017

4. TITLE AND SUBTITLE
Isolating Flow-field Discontinuities while Preserving Monotonicity and High-order Accuracy on Cartesian Meshes

5a. CONTRACT NUMBER

5b. GRANT NUMBER
N/A

5c. PROGRAM ELEMENT NUMBER
N/A

5d. PROJECT NUMBER
N/A

5e. TASK NUMBER
N/A

5f. WORK UNIT NUMBER
Q1FZ

6. AUTHOR(S)
Mundis, N., Lietz, C. and Sankaran, V.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQR
5 Pollux Drive
Edwards AFB, CA 93524-7048

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQR
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10. SPONSOR/MONITOR'S ACRONYM(S)
N/A

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-RQ-ED-VG-2017-001

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited. PA Case Number: 17030 Clearance Date: 17 January 2017
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13. SUPPLEMENTARY NOTES
For presentation at AIAA SciTech 2017; Grapevine, TX, USA (January 9-11, 2017)
Prepared in collaboration with Sierra Lobo and ERC

14. ABSTRACT
Viewgraph/Briefing Charts

15. SUBJECT TERMS
N/A

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON / 19b. TELEPHONE NUMBER *(Include area code)*
Unclassified	Unclassified	Unclassified	SAR	18	V. Sanakaran / N/A

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

Isolating Flow-field Discontinuities while Preserving Monotonicity and High-order Accuracy on Cartesian Meshes

Nathan L. Mundis – ERC, Inc.
Christopher F. Lietz – Sierra Lobo, Inc.
Venke Sankaran – AFRL/RQ

2017 AIAA SciTech
January 9, 2017

Introduction

- Filtering schemes offer a less dissipative alternative to the standard artificial dissipation operators when applied to high-order spatial/temporal schemes
- ***Limiting Fact:*** Filters impart the same amount of dissipation each time they are applied so if they are applied too frequently, they are overly dissipative
- ***Limiting Fact:*** Stiff systems require a preconditioned dual-time framework to be solved efficiently
- ***Limiting Fact:*** Filtering cannot be applied only at the physical-time level and convergence guaranteed
- ***Limiting Fact:*** Filtering cannot be straightforwardly applied at the pseudo-time level

Objective: To recast common filtering operators as equivalent artificial-dissipation schemes

Governing Equations

- **Navier-Stokes Equations:**

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H} \qquad \mathbf{Q} = [\rho \quad \rho u_i \quad \rho e_0]^{\mathsf{T}}$$

$$\mathbf{F}_i = [\rho u_i \quad \rho u_i u_j + p\delta_{ij} \quad u_i \rho h_0]^T \text{ where } h_0 = e_0 + \tfrac{p}{\rho}$$

- **Quasi-linear Form:**

$$\frac{\partial \mathbf{Q}}{\partial t} + \underline{\mathbf{A}}\frac{\partial \mathbf{Q}}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H} \qquad \underline{\mathbf{A}} = \tfrac{\partial \mathbf{F}_i}{\partial \mathbf{Q}} = \underline{\mathbf{M}\mathbf{\Lambda}\mathbf{M}}^{-1}$$

$$\underline{\mathbf{\Lambda}} = diag\left\{u_i + c, u_i, u_i - c\right\}$$

- **Primitive Variables Form:**

$$\underline{\mathbf{\Gamma}}_e \frac{\partial \mathbf{Q}_p}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H} \quad \Rightarrow \quad \underline{\mathbf{\Gamma}}_e \frac{\partial \mathbf{Q}_p}{\partial t} + \underline{\mathbf{A}\mathbf{\Gamma}}_e \frac{\partial \mathbf{Q}_p}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H}$$

$$\text{where } \underline{\mathbf{\Gamma}}_e = \tfrac{\partial \mathbf{Q}}{\partial \mathbf{Q}_p} \text{ and } \mathbf{Q}_p = [p \quad u_i \quad T]^{\mathsf{T}}$$

Governing Equations

- **Residual Form:**

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}_s\left(\mathbf{Q}\right) = \frac{\partial \mathbf{Q}_p}{\partial t} + \underline{\mathbf{\Gamma}}_e^{-1}\mathbf{R}_s\left(\mathbf{Q}_p\right) = 0 \qquad \text{where } \mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$

- **Temporal Discretizations:**
  - *SSPRK(3, 3):*

$$\begin{aligned}
\mathbf{Q}^{(1)} &= \mathbf{Q}^n - \Delta t \mathbf{R}_s\left(\mathbf{Q}^n\right) \\
\mathbf{Q}^{(2)} &= \frac{3}{4}\mathbf{Q}^n + \frac{1}{4}\left(\mathbf{Q}^{(1)} - \Delta t \mathbf{R}_s\left(\mathbf{Q}^{(1)}\right)\right) \\
\mathbf{Q}^{n+1} &= \frac{1}{3}\mathbf{Q}^n + \frac{2}{3}\left(\mathbf{Q}^{(2)} - \Delta t \mathbf{R}_s\left(\mathbf{Q}^{(2)}\right)\right)
\end{aligned}$$

$$\begin{aligned}
\mathbf{Q}_p^{(1)} &= \mathbf{Q}_p^n - \Delta t \mathbf{R}_{s,p}\left(\mathbf{Q}_p^n\right) \\
\mathbf{Q}_p^{(2)} &= \frac{3}{4}\mathbf{Q}_p^n + \frac{1}{4}\left(\mathbf{Q}_p^{(1)} - \Delta t \mathbf{R}_{s,p}\left(\mathbf{Q}_p^{(1)}\right)\right) \\
\mathbf{Q}_p^{n+1} &= \frac{1}{3}\mathbf{Q}_p^n + \frac{2}{3}\left(\mathbf{Q}_p^{(2)} - \Delta t \mathbf{R}_{s,p}\left(\mathbf{Q}_p^{(2)}\right)\right)
\end{aligned}$$

$$\text{where } \mathbf{R}_{s,p}\left(\mathbf{Q}_p^{(\ell)}\right) = \underline{\mathbf{\Gamma}}_e^{-1,(\ell)}\mathbf{R}_s\left(\mathbf{Q}_p^{(\ell)}\right)$$

  - *SSPRK(4, 3):*

$$\begin{aligned}
\mathbf{Q}^{(1)} &= \mathbf{Q}^n - \frac{1}{2}\Delta t \mathbf{R}_s\left(\mathbf{Q}^n\right) \\
\mathbf{Q}^{(2)} &= \mathbf{Q}^{(1)} - \frac{1}{2}\Delta t \mathbf{R}_s\left(\mathbf{Q}^{(1)}\right) \\
\mathbf{Q}^{(3)} &= \frac{2}{3}\mathbf{Q}^n + \frac{1}{3}\left(\mathbf{Q}^{(2)} - \frac{1}{2}\Delta t \mathbf{R}_s\left(\mathbf{Q}^{(2)}\right)\right) \\
\mathbf{Q}^{n+1} &= \mathbf{Q}^{(3)} - \frac{1}{2}\Delta t \mathbf{R}_s\left(\mathbf{Q}^{(3)}\right)
\end{aligned}$$

Spatial Discretizations

- **Discretely-conservative High-order Upwind using Roe's Approximate Riemann Solver:**

$$\frac{\partial \mathbf{F}_{i,j}}{\partial x_i} = \frac{\mathbf{F}_{i,j+1/2} - \mathbf{F}_{i,j-1/2}}{\Delta x_i} \qquad \text{where } \mathbf{F}_{i,j\pm 1/2} = \mathbf{F}_{LR} = f\left(\mathbf{Q}_L, \mathbf{Q}_R\right)$$

For instance, the standard second-order central difference can be found using:

$$\mathbf{F}_{+1/2} = \frac{\mathbf{F}(\mathbf{Q}_{+1}) + \mathbf{F}(\mathbf{Q}_0)}{2} \text{ and } \mathbf{F}_{-1/2} = \frac{\mathbf{F}(\mathbf{Q}_0) + \mathbf{F}(\mathbf{Q}_{-1})}{2}$$

- **High-order Interface States:**

$$\upsilon_{L,+1/2} = \frac{-\upsilon_{-1} + 5\upsilon_0 + 2\upsilon_{+1}}{6}$$

$$\upsilon_{R,+1/2} = \frac{-\upsilon_{+2} + 5\upsilon_{+1} + 2\upsilon_0}{6}$$

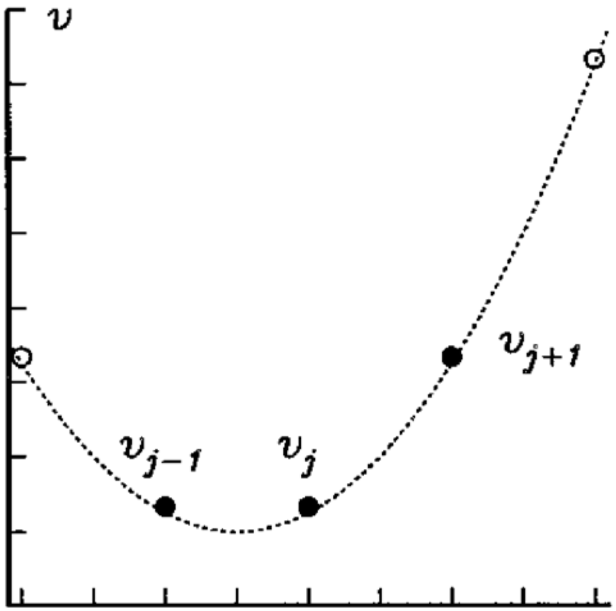
$$\upsilon_{L,+1/2} = \frac{2\upsilon_{-2} - 13\upsilon_{-1} + 47\upsilon_0 + 27\upsilon_{+1} - 3\upsilon_{+2}}{60}$$

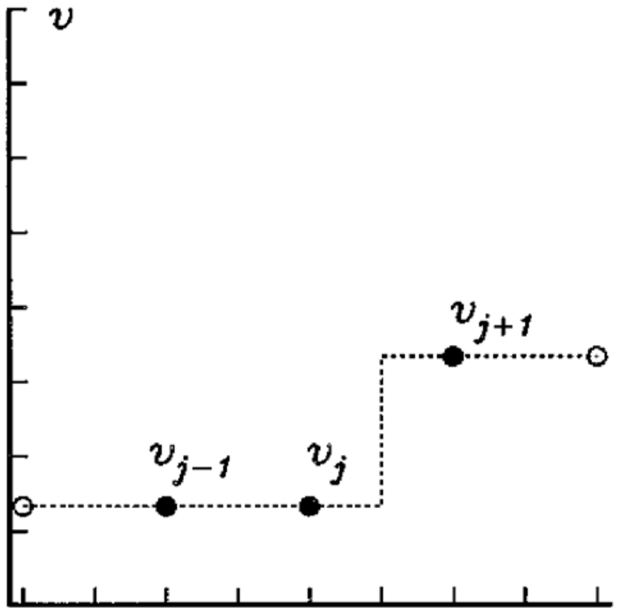
$$\upsilon_{L,+1/2} = \frac{-3\upsilon_{-3} + 25\upsilon_{-2} - 101\upsilon_{-1} + 319\upsilon_0 + 214\upsilon_{+1} - 38\upsilon_{+2} + 4\upsilon_{+3}}{420}$$

$$\upsilon_{L,+1/2} = \frac{4\upsilon_{-4} - 41\upsilon_{-3} + 199\upsilon_{-2} - 641\upsilon_{-1} + 1879\upsilon_0 + 1375\upsilon_{+1} - 305\upsilon_{+2} + 55\upsilon_{+3} - 5\upsilon_{+4}}{2520}$$

Limiter: Monotonicity-preserving Method

- **Limits the left and right interface quantities such that they are within an interval that is guaranteed to preserve monotonicity with an appropriate *CFL* number**
- **Uses a five-point stencil to distinguish between local extrema and discontinuities**





- **Further details are in the paper**

Limited Quantities

- **Either the conserved, the primitive, or the characteristic variables can be limited by the MP scheme**
- **Local characteristic limiting can be carried out as follows:**

For $\mathbf{Q}_{L,+1/2}$, the stencil consists of the set $\{\mathbf{Q}_{-2}, \mathbf{Q}_{-1}, \mathbf{Q}_{0}, \mathbf{Q}_{+1}, \mathbf{Q}_{+2}\}$.

$$\mathbf{W}_k = \underline{\mathbf{M}}_0^{-1}\mathbf{Q}_k \quad for \quad k = -2, 2$$
$$\mathbf{W}_{L,+1/2} = \underline{\mathbf{M}}_0^{-1}\mathbf{Q}_{L,+1/2}$$

$$\mathbf{Q}_{L,+1/2,\mathrm{lim}} = \underline{\mathbf{M}}_0\mathbf{W}_{L,+1/2,\mathrm{lim}}$$

or

$$\mathbf{W}_k = \underline{\mathbf{N}}_0^{-1}\mathbf{Q}_{p,k} \quad for \quad k = -2, 2$$
$$\mathbf{W}_{L,+1/2} = \underline{\mathbf{N}}_0^{-1}\mathbf{Q}_{p,L,+1/2}$$

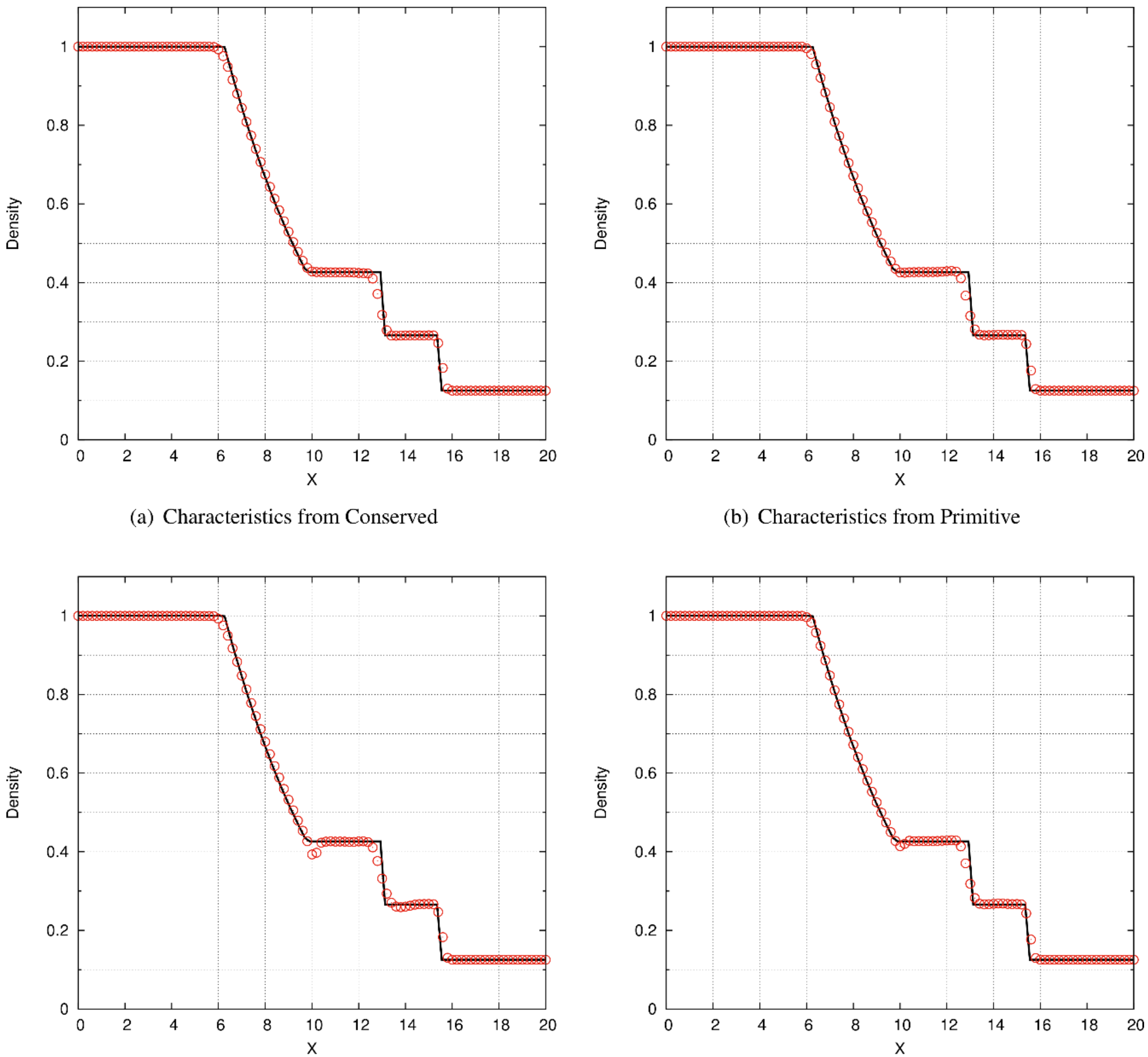
where $\underline{\mathbf{N}}^{-1} = \underline{\mathbf{M}}^{-1}\underline{\mathbf{\Gamma}}_e$. It is important to note that this necessarily implies that the same $\underline{\mathbf{\Gamma}}_e$ matrix (calculated at the midpoint of the set) resident in $\underline{\mathbf{N}}^{-1}$ is used for all five points in the limiting stencil.

Sod's Shock Tube Problem

- Domain 20 m long
- 100 points
- Discontinuity initially at x = 10 m
- Run for 50 time steps

$$\Delta t = 0.0002s$$
$$\sigma = 0.374$$
$$t_f = 0.01s$$

$$\begin{aligned} \rho_L &= 1.000, \rho_R = 0.125 \\ u_L &= 0.0, u_R = 0.0 \\ p_L &= 100000, p_R = 10000 \end{aligned}$$



(a) Characteristics from Conserved (b) Characteristics from Primitive

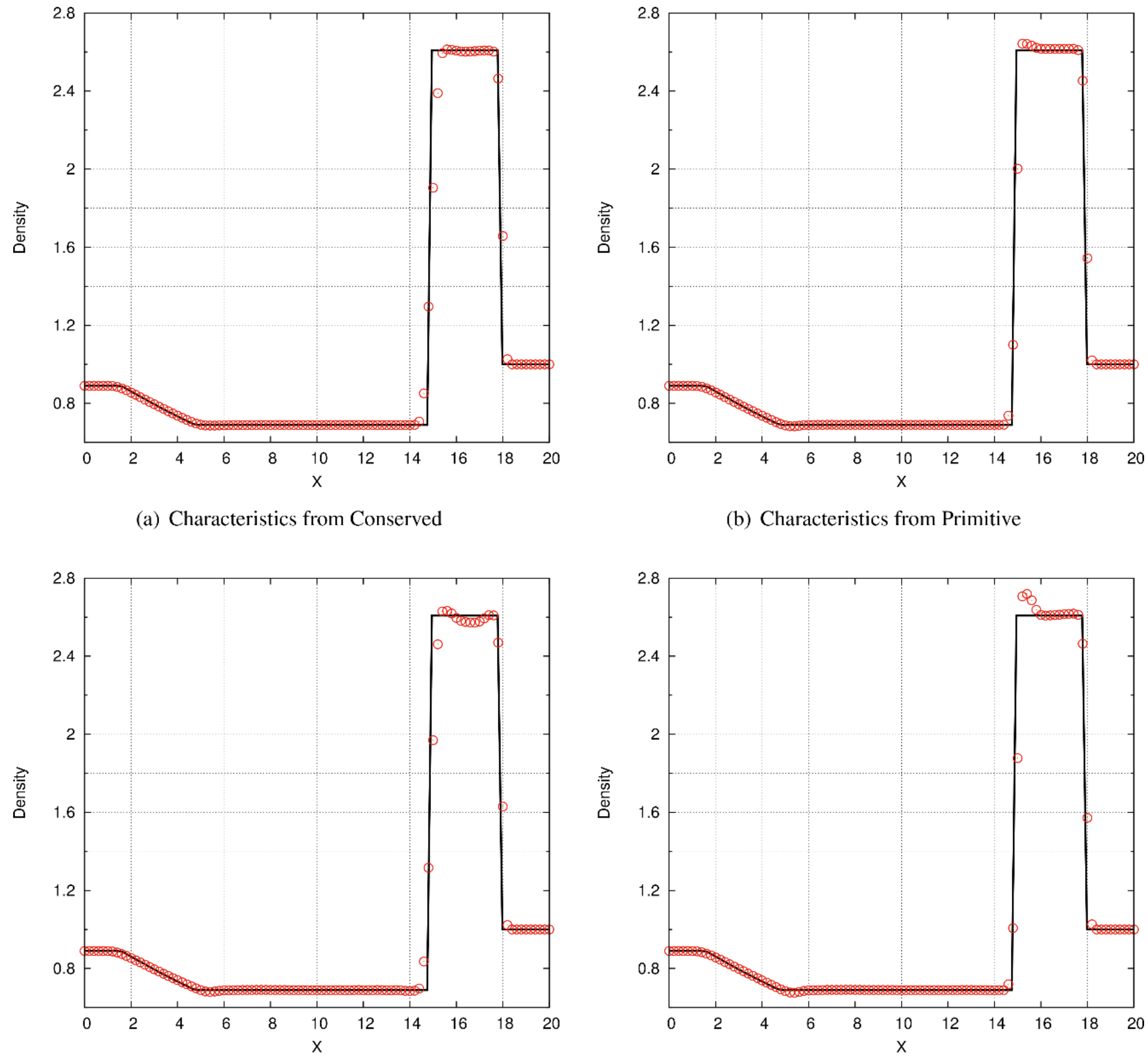
(c) Conserved (d) Primitive

Lax's Problem

- **Domain 20 m long**
- **100 points**
- **Discontinuity initially at x = 10 m**
- **Run for 160 time steps**

$$\Delta t = 0.0002s$$
$$\sigma = 0.403$$
$$t_f = 0.032s$$

$$\rho_L = 0.890, \rho_R = 1.000$$
$$u_L = 69.8, u_R = 0.0$$
$$p_L = 70560, p_R = 11420$$



(a) Characteristics from Conserved

(b) Characteristics from Primitive

(c) Conserved

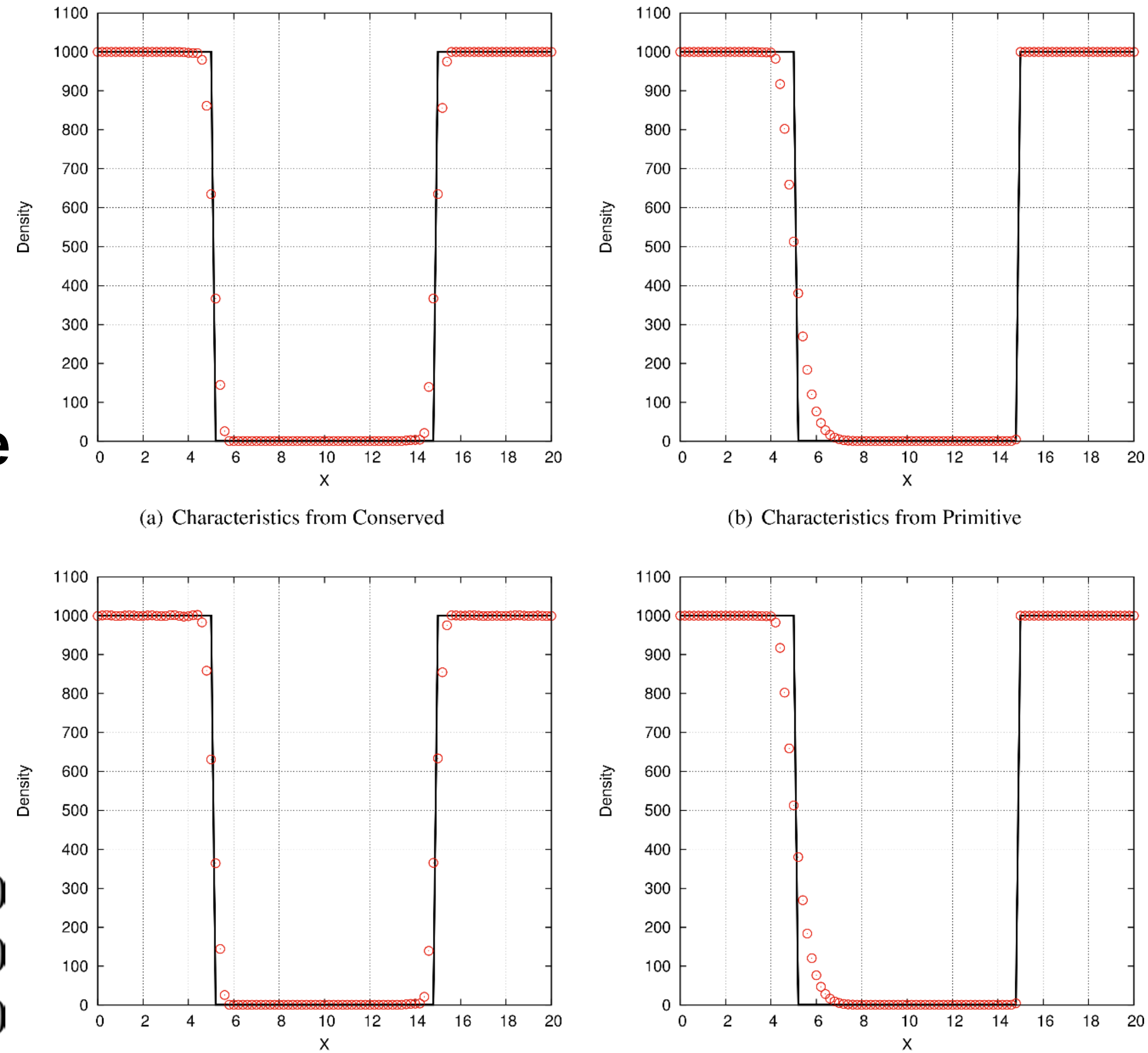
(d) Primitive

1D Contact Discontinuity Problem

- **Domain 20 m long**
- **100 points**
- **Discontinuities initially at x = 5 m and x = 15 m**
- **Run for 16,000 time steps**

$$\Delta t = 6.25 \times 10^{-5} s$$
$$\sigma = 0.370$$
$$t_f = 1.00 s$$

$$\rho_L = 1000,\ \rho_R = 1.00$$
$$u_L = 20.0,\ u_R = 20.0$$
$$p_L = 1000000,\ p_R = 1000000$$



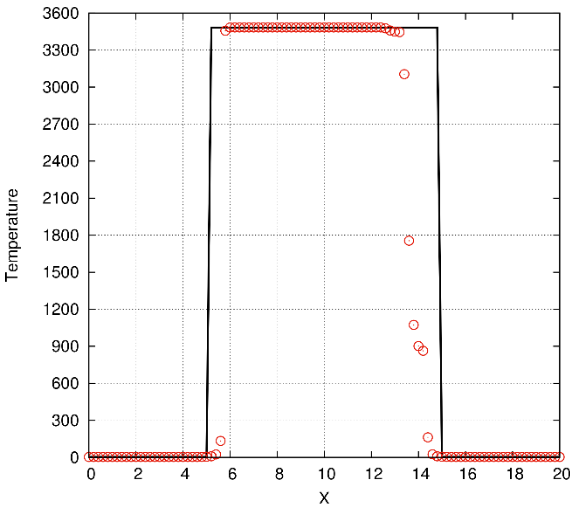
(a) Characteristics from Conserved

(b) Characteristics from Primitive

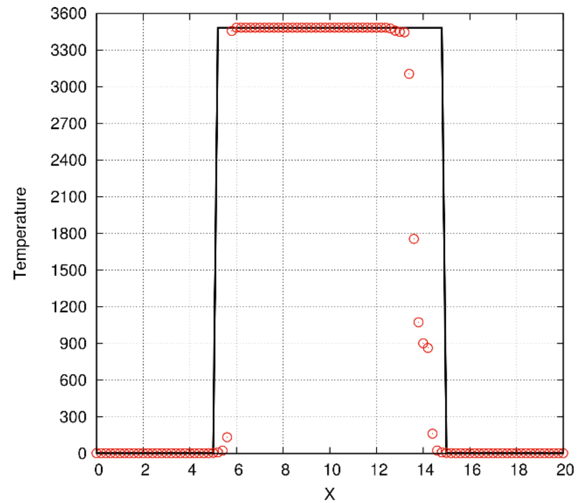
(c) Conserved

(d) Primitive

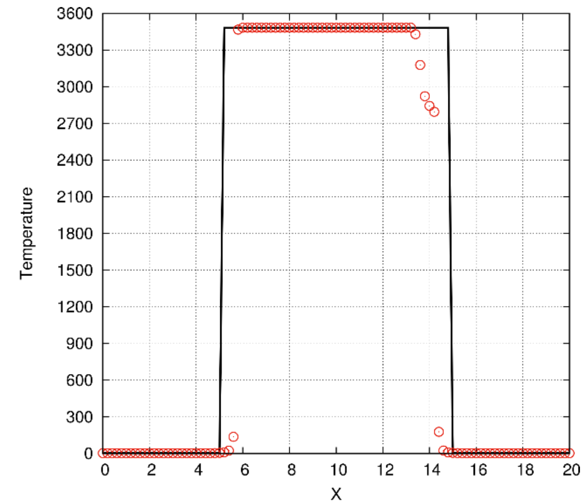
1D Contact Discontinuity Problem



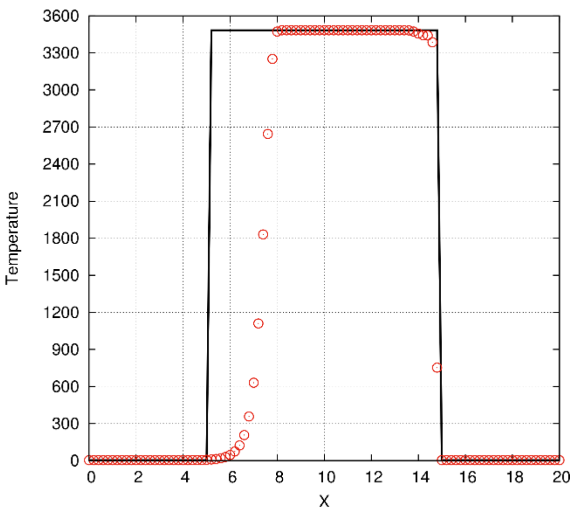
(a) Characteristics from Conserved



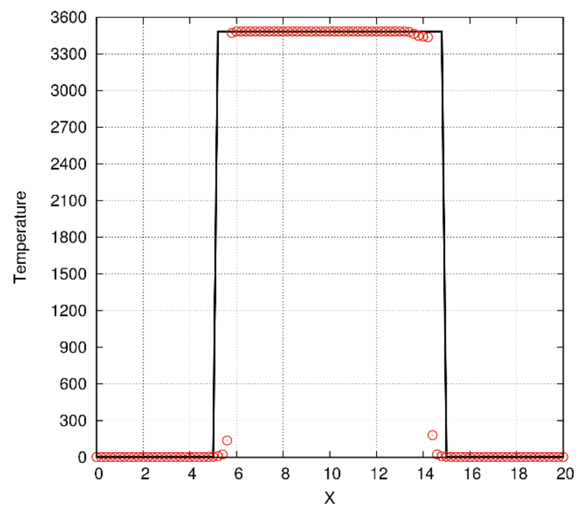
(a) $\alpha = 4$



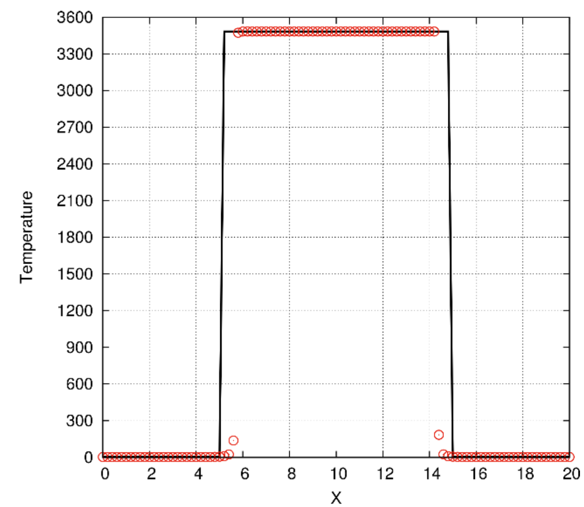
(b) $\alpha = 7$



(b) Characteristics from Primitive



(c) $\alpha = 11$



(d) $\alpha = 19$

2D Drop Problem

- **Domain 1 mm square**
- **100 points square**
- **Cold Fluid inside the drop**
- **Run for 25,000 time steps**

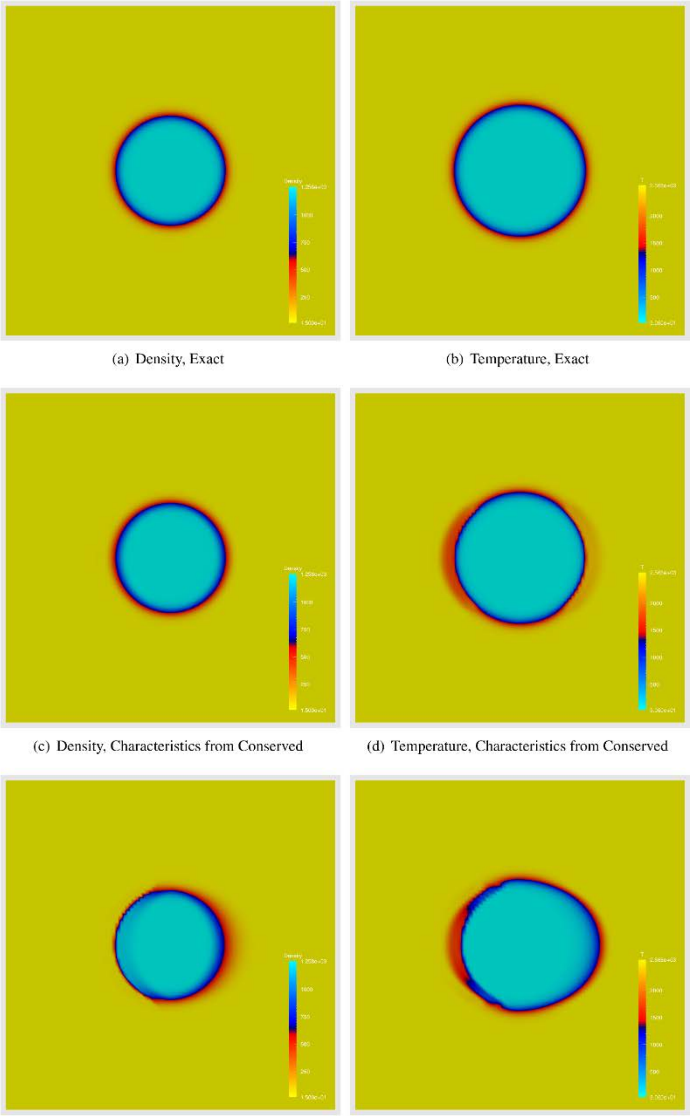
$$\Delta t = 4.0 \times 10^{-9} s$$
$$\sigma \approx 0.4$$
$$t_f = 1.0 \times 10^{-4} s$$

$$\rho_L = 15, \rho_R = 1258$$
$$u_L = 10.0, u_R = 10.0$$
$$p_L = 1 \times 10^7 \; p_R = 1 \times 10^7$$

$$\mathbf{Q} = \mathbf{Q}_R F + \mathbf{Q}_L (1 - F)$$

$$F = \frac{1}{2}\left[1 - \tanh\left(\frac{r - r_d}{\Delta_d}\right)\right]$$

$$r_d = 0.2mm \text{ and } \Delta_d = 0.015mm$$

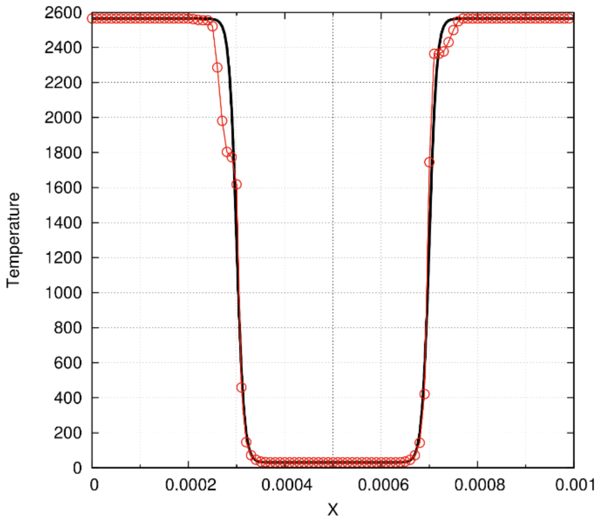


(a) Density, Exact (b) Temperature, Exact

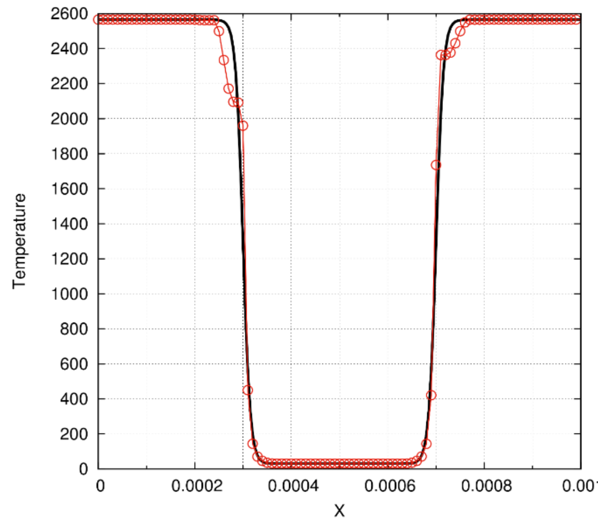
(c) Density, Characteristics from Conserved (d) Temperature, Characteristics from Conserved

(e) Density, Characteristics from Primitive (f) Temperature, Characteristics from Primitive

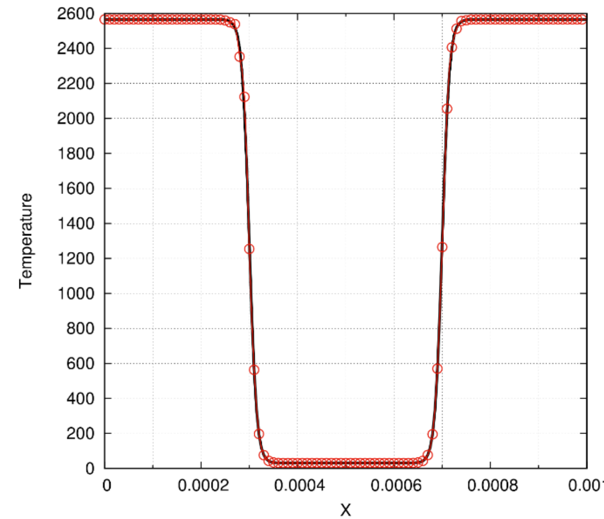
2D Drop Problem, Centerline T



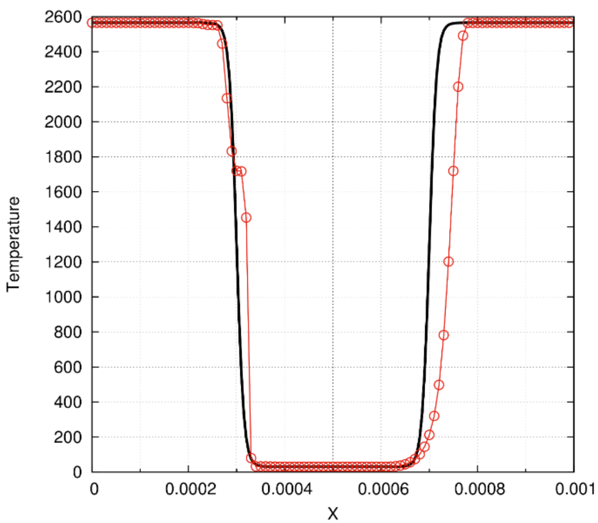
(a) Characteristics from Conserved



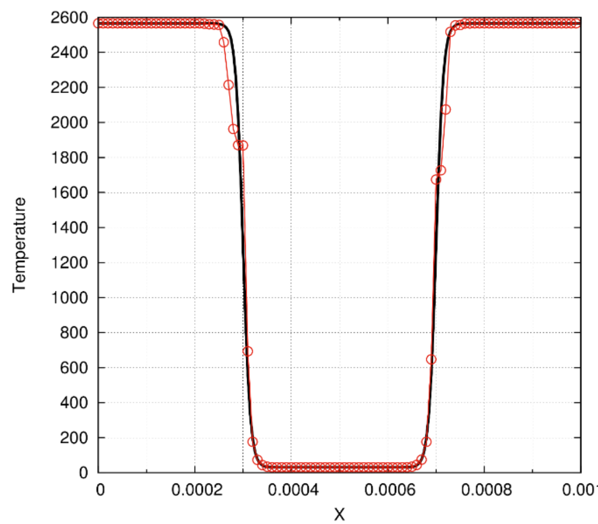
(a) $\alpha = 19$



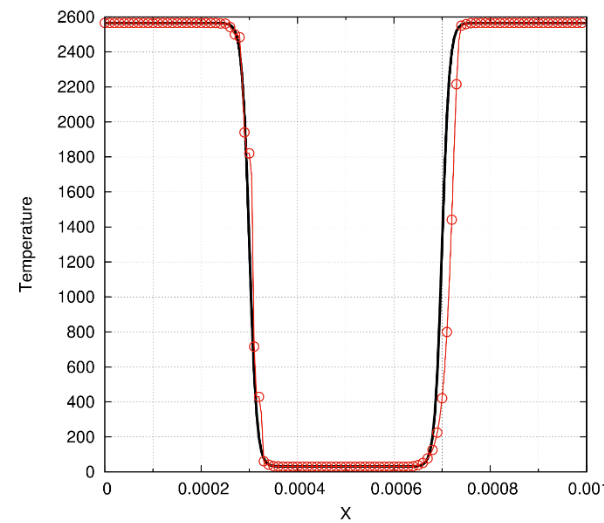
(a) Characteristics from Conserved, 2× Resolution



(b) Characteristics from Primitive



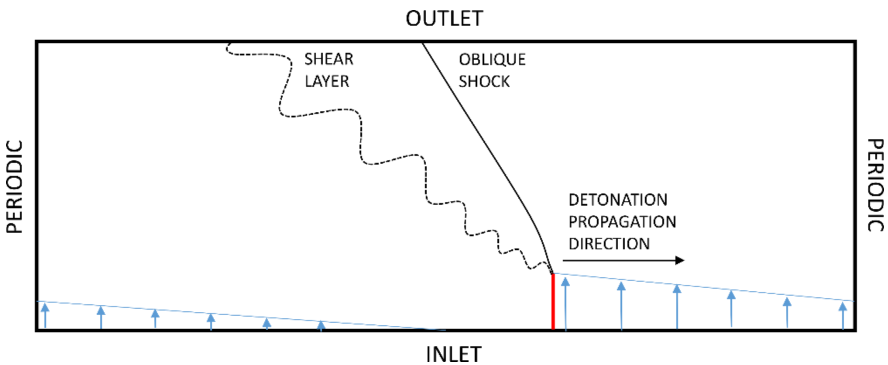
(b) $\alpha = 19$, Ninth-order

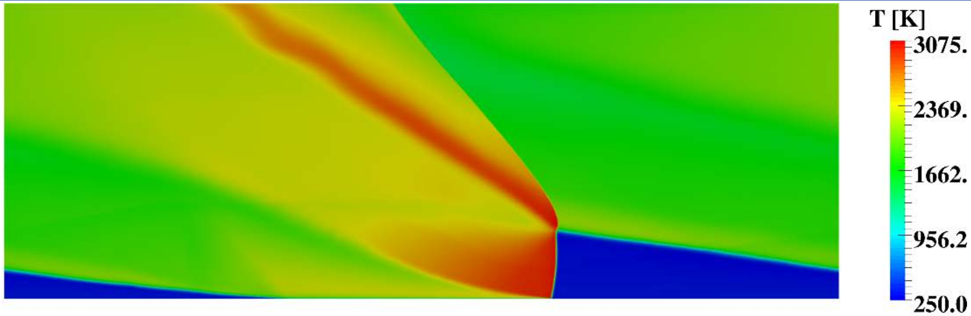


(b) Characteristics from Primitive, 2× Resolution

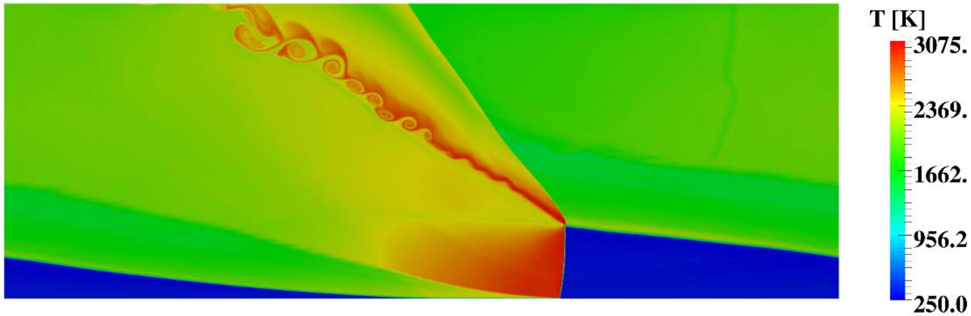
2D Rotating Detonation Wave

- **Unwrapped cylinder**
- **Follows the work of Schwer (reference in paper)**
- **Stoichiometric H_2/Air**
- p_{plenum} **= 10 ATM**
- T_{plenum} **= 300K**

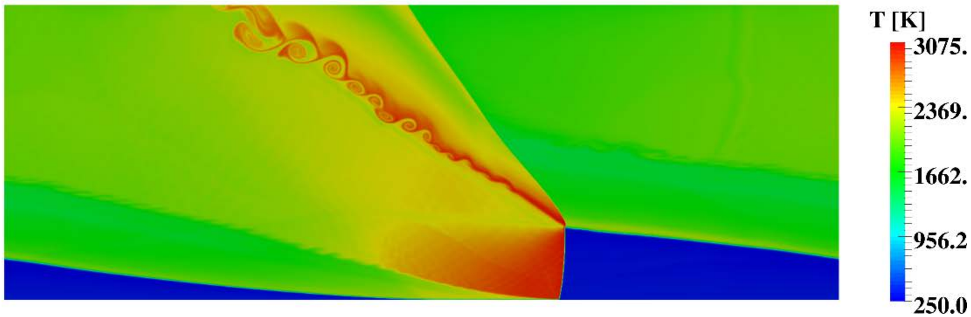




(a) Limit All Primitives



(b) Limit Non-monotone Primitives



(c) Limit Non-Monotone Characteristics From Primitives

Conclusions

- Applying existing high-order monotonicity-preserving methods to the primitive variables is not straightforward
- The MP scheme should be applied to the characteristic variables calculated from the conserved variables for the best results
- These results will offer unique results for more-complicated equations of state (EoS) where temperature and pressure cannot be calculated from density and internal energy directly

Future Work

- **Use a detection strategy to limit the frequency with which the limiter and, with it, the conversion from conserved to primitive via the EoS is applied**
  - Interpolate primitive variables
  - Detect where limiting might be needed
  - Only where needed, calculate characteristic variables from conserved variables
  - Note specifically where the MP limiter is active
  - Convert back to primitive variables only where the limiter is active
  - Use the first-order accurate value for the initial guess of temperature and pressure in the EoS routine
- **In this way, efficiency and accuracy can be optimized**

Questions???